

A Posteriori Error Bounds for Two Point Boundary Value Problems: A Green's Function Approach

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Abstract

We present a computer assisted method for generating existence proofs and a posteriori error bounds for solutions to two point boundary value problems (BVPs). All truncation errors are accounted for and, if combined with interval arithmetic to bound the rounding errors, the computer generated results are mathematically rigorous. The method is formulated for n -dimensional systems and does not require any special form for the vector field of the differential equation. It utilizes a numerically generated approximation to the BVP fundamental solution and Green's function and thus can be applied to stable BVPs whose initial value problem is unstable. The utility of the method is demonstrated on a pair of singularly perturbed model BVPs and by using it to rigorously show the existence of a periodic orbit in the Lorenz system.

Keywords: two point boundary value problems, computer assisted proofs, periodic orbits, a posteriori error analysis, singular perturbations

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1. Introduction

We propose a new computer assisted method for rigorously proving invertibility and bounding the norm of the inverse of operators of the form²

$$F[v](t) = \left(v(t) - v(0) - \int_0^t A(s)v(s)ds, B_0v(0) + B_1v(1) \right), \quad A(t), B_i \in \mathbb{R}^{n \times n}. \quad (1)$$

Operators of this form correspond to linear two point boundary value problems (BVPs) and arise naturally as the Fréchet derivative of operators defining nonlinear BVPs. Bounds on the norm of the inverse of operators of this type are required in a posteriori proofs of existence and local uniqueness of nonlinear equations via the Newton-Kantorovich theorem [15].

Computer assisted methods have been successfully applied to many problems in differential equations and dynamical systems, including chaos in the Rössler [41] and Lorenz [11] systems, the existence of the Lorenz attractor [35], flow (in)stability [4, 39], existence of heteroclinic [20], homoclinic [37, 1, 2], and periodic [5, 13] orbits, solution of the Feigenbaum equation [18], and the (in)stability of matter [7]. Generalizations to elliptic and parabolic PDEs are discussed in, for example, [26, 25, 28, 31]. As it pertains to two point boundary value problems, computer assisted proofs are typically based on a fixed point theorem [40, 30, 27]. In particular, various forms of the Newton-Kantorovich theorem

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²Conditions on $A(t)$ and the precise functions spaces in which we work will be specified later.

were used in [22, 17, 33]. A method based on differential inequalities as presented in [12], a method using radii polynomials is given in [13], and [21] utilized Chebyshev series.

The methods in [22, 12, 30, 33, 27, 9, 8] focused on second order equations; [22] worked with an equivalent integral formulation while [33, 27] used a finite element based method. [8] treated an integral boundary condition. The results in [36, 17] utilized the theory of initial value problem (IVP) fundamental solutions to treat n -dimensional two point BVPs, the former focusing on the periodic case.

Our method most closely resembles that of Ref. [17] and applies to n -dimensional systems without any special assumptions on the form of the vector field. The present method differs from [17] in the use of the BVP fundamental solution and Green's function as the primary tool, as opposed to the IVP fundamental solution. See also [38], which used a Green's function method to solve a singular problem on an unbounded domain.

A general outline of our method is as follows.

1. Generate (non-rigorous) approximations, $\tilde{\Phi}_j, \tilde{G}_{i,j}$ to the BVP fundamental solution and Green's function, respectively, on a mesh.
2. Extend these to piecewise polynomial approximations $\tilde{\Phi}(t)$ and $\tilde{G}(t, s)$ on the whole domain.
3. Use $\tilde{\Phi}$ and \tilde{G} to define an approximate inverse, H , to the BVP operator F .
4. Using estimates involving H , prove existence of an exact inverse to F and derive a machine computable formula that bounds the norm of F^{-1} .

The use of the BVP fundamental solution makes the method presented here applicable in a range of situations for which IVP based methods are ill suited, namely when the IVP fundamental solution or its inverse has a 'large' norm but the corresponding BVP fundamental solution and Green's function has a 'moderately sized' norm. This is often the case in singularly perturbed problems and so the effectiveness of the method is demonstrated on two such examples in section 9. We will refer to these imprecisely defined 'large' and 'moderate' regimes as unstable and stable respectively, similar to the discussion in [3].

To obtain completely rigorous results, some means of bounding the floating point rounding error is needed, typically based on the theory of interval arithmetic. There are many references from which to learn more about validated numerics and interval arithmetic, for example [23, 16, 14, 24, 34]. Results in this paper are presented so that if interval arithmetic is used for all arithmetic operations and interval valued extensions are available for the vector field of the differential equation and its derivatives then the resulting computer generated existence proofs and error bounds are mathematically rigorous (we use the MATLAB package INTLAB [32] to obtain rigorous bounds). However, in light of the additional computational cost of interval arithmetic as compared to floating point, if complete rigor is not needed then the method can just as easily be used with traditional floating point operations to obtain approximate error bounds.

In section 2 we fix some notation and discuss a general strategy for a posteriori existence proofs via the Newton-Kantorovich theorem. For comparison, we outline the method of [17] in section 3. Development of our method begins in section 4 and continues in subsequent sections. Background on the Green's function of a BVP is given in section 5. The method is tested on several sample problems in section 9.

2. A Posteriori Existence Proofs via Newton-Kantorovich

Consider a general non-linear two point BVP on $[0, 1]$,

$$y'(t) = f(t, y(t)), \quad g(y(0), y(1)) = 0, \quad (2)$$

where $f : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ is continuous, differentiable in y , $D_y f$ is continuous on \mathbb{R}^{n+1} , and $g : \mathbb{R}^{2n} \rightarrow \mathbb{R}^n$ is C^1 . In particular, local existence and uniqueness of the IVP is guaranteed.

In order to apply functional analytic methods to this problem it is convenient to follow [17] and define the Banach spaces

$$X_1 = C([0, 1], \mathbb{R}^n), \quad C_0([0, 1], \mathbb{R}^n) \equiv \{y \in X_1 : y(0) = 0\}, \quad X_2 = C_0([0, 1], \mathbb{R}^n) \times \mathbb{R}^n \quad (3)$$

where the ∞ -norm is used on \mathbb{R}^n , denoted by $|\cdot|$, the sup-norm $\|y\| \equiv \sup_{[0,1]} |y(t)|$ is used on the function spaces, and the norm $\|(y, b)\| = \max\{\|y\|, |b|\}$ is used on X_2 .

In this setting, the BVP (2) can be put in a form more amenable to analysis as follows. Define the map $G : X_1 \rightarrow X_2$

$$G[y](t) = \left(y(t) - y(0) - \int_0^t f(s, y(s)) ds, g(y(0), y(1)) \right). \quad (4)$$

Solutions of the BVP are in one to one correspondence with zeros of G . Its first component, valued in $C_0([0, 1], \mathbb{R}^n)$, is denoted by G^1 and its second component, valued in \mathbb{R}^n , by G^2 . As shown in [17], G is Fréchet- C^1 with derivative at $y_0 \in X_1$ given by

$$\begin{aligned} DG^1(y_0)[v](t) &= v(t) - v(0) - \int_0^t D_y f(s, y_0(s)) v(s) ds, \\ DG^2(y_0)[v](t) &= D_{y_1} g(y_0(0), y_0(1)) v(0) + D_{y_2} g(y_0(0), y_0(1)) v(1). \end{aligned} \quad (5)$$

Having reformulated the problem in terms of finding zeros of a C^1 map between Banach spaces, a natural tool is the Newton-Kantorovich theorem; see Appendix Appendix A for a precise statement. Invertibility of $DG(y_0)$ along with a bound on the norm of its inverse are required to apply the theorem and these are typically the most difficult ingredients to obtain in practice. Once this has been done the remainder of the estimates are relatively straightforward and have been discussed in, for example, [17]. For this reason we will predominately focus on the invertibility of $DG(y_0)$ i.e. on a posteriori methods for proving the existence and uniqueness to solutions of linear BVPs.

3. IVP Fundamental Solution Method

Motivated by the previous section, consider a linear BVP on $[0, 1]$ as given by the bounded linear operator $F : X_1 \rightarrow X_2$ defined by the formula (1), where $A(t)$ is a continuous $\mathbb{R}^{n \times n}$ valued map.

In Theorem 1 of [17], the author shows how the solvability of $F[v] = (r, w)$ is related to the matrix of fundamental solutions, defined as the solution to the initial value problem (IVP)

$$Y'(t) = A(t)Y(t), \quad Y(0) = I.$$

In our notation, this result is the following.

Theorem 1. *Let $A(s)$ and $r(t)$ be continuous matrix and vector valued respectively with $r(0) = 0$ and consider the two point BVP*

$$v(t) = v(0) + \int_0^t A(s)v(s) ds + r(t), \quad B_0 v(0) + B_1 v(1) = w.$$

Let $Y(t)$ be the corresponding matrix of fundamental solutions and define $R = B_0 + B_1 Y(1)$. Then the BVP has a unique solution iff R is nonsingular and the solution is

given by

$$v(t) = Y(t) \left[R^{-1} B_0 \int_0^t Y^{-1}(s) A(s) r(s) ds + (R^{-1} B_0 - I) \int_t^1 Y^{-1}(s) A(s) r(s) ds - R^{-1} (B_1 r(1) - w) \right] + r(t).$$

It was also shown in [17] how to apply this theorem to rigorously prove solvability of the BVP and derive guaranteed error bounds using numerically constructed approximations to $Y(t)$ and $Y^{-1}(t)$. Because of the use of Y , this will be called the IVP fundamental solution method or simply the IVP method.

A limitation of this method is that the stability properties of an IVP take center stage; the quantities $|Y(t)|$ and $|Y^{-1}(t)|$ feature critically in the error estimates derived in [17]. Unfortunately there are situations in which a BVP of interest is stable whereas the corresponding IVP is not. In such situations the bounds obtained by the IVP fundamental solution method will be very pessimistic due to the large size of $|Y(t)|$ and/or $|Y^{-1}(t)|$.

As discussed in [3], perhaps the simplest test problem that exhibits these features is the BVP

$$y''(t) = y(t) \quad y(0) = 1, \quad y(b) = 0. \quad (6)$$

The corresponding IVP fundamental solution matrix and its inverse are

$$Y(t) = \begin{pmatrix} \cosh(t) & \sinh(t) \\ \sinh(t) & \cosh(t) \end{pmatrix}, \quad Y^{-1}(t) = \begin{pmatrix} \cosh(t) & -\sinh(t) \\ -\sinh(t) & \cosh(t) \end{pmatrix}.$$

These have exponentially increasing norms as a function of b . This is in spite of the fact that the value and derivative of the exact solution

$$y(t) = \cosh(t) - \cosh(b) \sinh(t) / \sinh(b)$$

have $\mathcal{O}(1)$ norm.

Even if one tries to avoid separately bounding the norms of Y and Y^{-1} and take advantage of the cancellation that can occur in $Y(t)R^{-1}B_0Y^{-1}(s)$ and $Y(t)(R^{-1}B_0 - I)Y^{-1}(s)$, the above example is sufficient to show that this cancellation does not in general occur over the entire (t, s) domain; the 1, 1 component of the former quantity is given by

$$(Y(t)R^{-1}B_0Y^{-1}(s))_1^1 = (\cosh(t) - \cosh(b) \sinh(t) / \sinh(b)) \cosh(s)$$

which diverges at $t = 0, s = b$ as $b \rightarrow \infty$. Even if cancellation does occur, it is difficult to compute $Y(t)$ and $Y^{-1}(s)$ to high enough accuracy that one could take advantage of such cancellation.

In summary, while the IVP fundamental solution method suffices for problems whose IVP is stable, if one is interested in BVPs whose corresponding IVP is unstable then an alternative method is needed. Our contribution is designed to address such situations by utilizing the BVP fundamental solution and Green's function in place of the IVP fundamental solution.

4. A More General Framework

We are now in position to begin discussing an alternative method for producing a posteriori existence proofs and error bounds based on the BVP fundamental solution. This method will be called the BVP fundamental solution method, or BVP method for

short, in contrast to the IVP method. The BVP fundamental solution is introduced in the following section, but first we discuss the function spaces that will be used in our analysis.

The input to any a posteriori method consists of a certain (numerically generated) approximate solution. For us this will consist of function values on a mesh $0 = t_0 < \dots < t_N = 1$. Before error bounds can be produced, these need to be extended to an approximate solution on the entire interval $[0, 1]$. While one could work in spaces of continuous functions by interpolating the values at the nodes, as done in the IVP method, we will find things more convenient (and the resulting error bounds more transparent) when this assumption is removed, both from the solution space and the matrix $A(t)$. In this section we outline the slightly generalized framework in which the equations will be formulated.

To this end, fix a mesh, t_i , as above and let Y_1 be the space of functions that are piecewise continuous on this mesh. More precisely, Y_1 is the direct sum

$$Y_1 = \bigoplus_{j=1}^N C([t_{j-1}, t_j], \mathbb{R}^n). \quad (7)$$

On each factor the norm will be taken to be a weighted ∞ -norm

$$\|(v_1, \dots, v_N)\|_W \equiv \max_{j=1, \dots, N} \|v_j\|_j, \quad \|v_j\|_j \equiv \sup_{t \in [t_{j-1}, t_j]} |v_j(t)|_W, \quad |v_j|_W \equiv |W v_j|$$

where the weight, W , is some invertible matrix. In practice, we will take W to be diagonal and choose the diagonal elements to balance the magnitude of the errors in the different components of the solution. One could consider the generalization where the weight is allowed to vary between subintervals but this will not be explored here.

Y_1 is a Banach space and the maps that send any $y \in Y_1$ to its value at any $t \in \{0, 1\} \cup \bigcup_{j=1}^N (t_{j-1}, t_j)$ or at t_j^\pm ($+$ denotes limit from above, $-$ limit from below) are well defined bounded linear maps. Elements of Y_1 can be identified with elements of L^∞ and integration or differentiation (of piecewise C^1) elements of Y_1 will be defined using this identification.

Mirroring the continuous case, (3), define a second space

$$Y_2 = \{v \in Y_1 : v(0) = 0\} \times \mathbb{R}^n. \quad (8)$$

This is a Banach space under the norm $\|(v, b)\|_{W_1, W_2} = \max\{\|v\|_{W_1}, |b|_{W_2}\}$ where W_i are any invertible matrices. Finally, note that the X_i 's are closed subspaces of the Y_i 's. For simplicity we will take $W_1 = W_2 = W$. This will allow us to drop the subscript W 's from the above norms in the following sections.

Having specified the functional analytic framework, the definition of nonlinear BVPs can be extended to this setting by defining $G : Y_1 \rightarrow Y_2$ by the same formula as in (4). Note that any zero of this map is automatically continuous, and so solutions of the generalized problem are still in 1-1 correspondence with solutions of the original BVP.

The extended operator G is still Fréchet- C^1 , with the same formula for the derivative (5). Note, however, that $D_y f(s, y_0(s))$ is no longer continuous as a function of s for a general $y_0 \in Y_1$. Therefore, in the interest of applying Newton-Kantorovich to prove existence, we are lead to consider bounded linear maps $F : Y_1 \rightarrow Y_2$ defined as in (1), where the assumptions on $A(s)$ are relaxed to allow for piecewise continuity on the given mesh.

5. Green's Function for Linear BVPs

We are now in position to discuss the BVP fundamental solution, on which our method will be based. A BVP fundamental solution is defined as a continuous and piecewise C^1

solution to

$$\Phi' = A\Phi, \quad B_0\Phi(0) + B_1\Phi(1) = I$$

consisting of invertible matrices. Recall that $A(t)$ is only assumed to be piecewise continuous. Analogously to the IVP fundamental solution, if a BVP fundamental solution exists then it provides an inverse to the BVP operator F through the Green's function, as defined in the following theorem.

Theorem 2. *If a BVP fundamental solution Φ exists then it is unique and the unique solution to*

$$v(t) - v(0) - \int_0^t A(s)v(s)ds = r(t), \quad B_0v(0) + B_1v(1) = w$$

can be written

$$v(t) = \Phi(t)(w - B_1r(1)) + r(t) + \int_0^1 G(t,s)A(s)r(s)ds$$

where the Green's Function is defined as

$$G(t,s) = \begin{cases} \Phi(t)B_0\Phi(0)\Phi^{-1}(s), & \text{if } s \leq t \\ -\Phi(t)B_1\Phi(1)\Phi^{-1}(s), & \text{if } s > t. \end{cases} \quad (9)$$

Therefore Φ provides us with an inverse of the operator F from (1) given by

$$F^{-1} : (r(t), w) \rightarrow \Phi(t)(w - B_1r(1)) + r(t) + \int_0^1 G(t,s)A(s)r(s)ds. \quad (10)$$

Note that the Green's function (9) is not to be confused with the notation for the operator associated with a nonlinear BVP (4). The meaning will be clear from the context.

Theorem 2 is essentially found in [3]. The only complications beyond the presentation there is that $A(t)$ is only piecewise continuous and $r(t)$ must be taken to be an arbitrary continuous function that vanishes at $t = 0$, not necessarily one of the form

$$r(t) = \int_0^t q(s)ds$$

for some continuous q , as would be the case when transforming from the differential to the integral form of the BVP. One can directly verify the formula by composing (10) with (1) and vice versa.

6. Proving Invertibility

We now suppose that we are given piecewise C^1 maps

$$\tilde{\Phi} : [0, 1] \rightarrow \mathbb{R}^{n \times n}, \quad \tilde{G} : [0, 1] \times [0, 1] \rightarrow \mathbb{R}^{n \times n},$$

which are thought of an approximate fundamental BVP solution and approximate Green's function respectively (but without any a priori knowledge that an exact Φ actually exists) which were obtained by non-rigorous numerical means. More specifically, there are a set of nodes $0 = t_0 < \dots < t_N = 1$ such that each $\tilde{\Phi}|_{[t_{i-1}, t_i]}$ is C^1 and each $\tilde{G}|_{[t_{i-1}, t_i] \times [t_{j-1}, t_j]}$ is C^1 , except when $i = j$, in which case \tilde{G} also has a discontinuity along the diagonal. We will construct \tilde{G} using $\tilde{\Phi}$ and an approximation to its inverse by replacing the corresponding exact quantities in the definition of the Green's function (9), but this is not strictly necessary.

Our strategy for proving the existence of $F^{-1} : Y_2 \rightarrow Y_1$ is to mimic the formula (10) for $F^{-1} : X_2 \rightarrow X_1$ in terms of the fundamental solution but using the approximate fundamental solution instead. More precisely, replacing Φ with $\tilde{\Phi}$ and G with \tilde{G} in the formula for F^{-1} yields a bounded linear map $H : Y_2 \rightarrow Y_1$.

H will be used to find conditions under which we can prove the invertibility of F . This will rely on the following well known result concerning perturbations of the identity, see for example [10].

Lemma 3. *Let $A : X \rightarrow X$ be a bounded linear map on a Banach space. If $\|I - A\| < 1$ then A has a bounded inverse that satisfies*

$$\|A^{-1}\| \leq \frac{1}{1 - \|I - A\|}.$$

In fact, a slight generalization of this result will be needed, given below.

Lemma 4. *Let $A : X \rightarrow Y$, $B : Y \rightarrow X$ be bounded linear maps where X, Y are Banach spaces. If $\|I - AB\| \leq \alpha$ for $\alpha < 1$ where I is the identity on Y then A is surjective. If A is also injective then A, B are invertible,*

$$\|A^{-1}\| \leq \frac{\|B\|}{1 - \alpha} \text{ and } \|A^{-1} - B\| \leq \frac{\alpha\|B\|}{1 - \alpha}.$$

PROOF. By the above lemma, AB has a bounded inverse with

$$\|(AB)^{-1}\| \leq \frac{1}{1 - \|I - AB\|} \leq \frac{1}{1 - \alpha}.$$

In particular A is surjective. It is injective by assumption so by the open mapping theorem it has a bounded inverse. This implies B has a bounded inverse as well and

$$\|A^{-1}\| = \|BB^{-1}A^{-1}\| = \|B(AB)^{-1}\| \leq \frac{\|B\|}{1 - \alpha},$$

$$\|A^{-1} - B\| = \|A^{-1}(I - AB)\| \leq \|A^{-1}\|\|I - AB\| \leq \frac{\alpha\|B\|}{1 - \alpha}.$$

6.1. Applying the Fredholm Alternative

In finite dimensions and when X and Y have the same dimension then the hypothesis of injectivity of A in Lemma 4 is not needed but in infinite dimensions it is required in general. However, when we have the appropriate element of compactness, the situation in infinite dimensions mirrors the finite dimensional case. More specifically, recall one consequence of the Fredholm alternative, see for example [6].

Theorem 5. *Let X be a Banach space and $K : X \rightarrow X$ be a compact operator. Then $I - K$ is injective iff it is surjective.*

If a Fredholm alternative-like condition holds for F then surjectivity will imply injectivity, and hence $\|I - FH\| < 1$ will imply the invertibility of F . In addition, this will provide a bound on F^{-1} per Lemma 4. These are the two ingredients that are needed in order to utilize the Newton-Kantorovich theorem. With slight modifications of the above we could just as well work with $I - HF$ but find this less appealing for a reason we point out in Appendix Appendix C.

In order to more easily apply the Fredholm alternative, we reformulate the BVP operator F in terms of a map from a single Banach space to itself. Define $\tilde{F} : Y_2 \rightarrow Y_2$

by

$$\begin{aligned}\tilde{F}[v, w](t) &= \left(v(t) - \int_0^t A(s)(w + v(s))ds, B_0 w + B_1(w + v(1)) \right) \\ &= (v(t), w) - \left(\int_0^t A(s)(w + v(s))ds, (I - B_0 - B_1)w - B_1 v(1) \right) \\ &\equiv (I - K)[v, w](t).\end{aligned}$$

We have $F[v] = \tilde{F}[v - v(0), v(0)]$ and so F is surjective or injective if and only if \tilde{F} is.

The second component of K has finite rank and the first is an integral operator with bounded kernel over a bounded domain and whose image consists of continuous functions, hence the compactness of K follows from an application of the Arzela-Ascoli theorem. This implies that the Fredholm alternative applies to \tilde{F} and hence, showing that $\|I - FH\| \leq \alpha < 1$ is sufficient to prove that F has a bounded inverse with

$$\|F^{-1}\| \leq \frac{\|H\|}{1 - \alpha}, \quad \|F^{-1} - H\| \leq \frac{\alpha\|H\|}{1 - \alpha}. \quad (11)$$

We will now discuss how to bound $\|I - FH\|$ and $\|H\|$.

6.2. Bounding $\|I - FH\|$

In Appendix Appendix B a formula for $I - FH$ is derived. For each $t \notin \{t_i\}_{i=0}^N$ let $j_t = \max\{j : t_j < t\}$. The two components of $I - FH$ are given by

$$\begin{aligned}(I - FH)[r, w]_1(t) &= - \int_0^t \tilde{\Phi}'(s) - A(s)\tilde{\Phi}(s)ds(w - B_1 r(1)) + \int_0^t (\tilde{G}(z^-, z) - \tilde{G}(z^+, z) + I)A(s)r(s)ds \\ &\quad + \sum_{j=1}^{j_t} (\tilde{\Phi}(t_j^-) - \tilde{\Phi}(t_j^+))(w - B_1 r(1)) + \int_0^1 \left[\sum_{j=1}^{j_t} (\tilde{G}(t_j^-, z) - \tilde{G}(t_j^+, z)) \right] A(z)r(z)dz \\ &\quad - \int_0^t \int_0^1 (\partial_s \tilde{G}(s, z) - A(s)\tilde{G}(s, z))A(z)r(z)dzds, \\ (I - FH)[r, w]_2 &= [I - B_0 \tilde{\Phi}(0) - B_1 \tilde{\Phi}(1)](w - B_1 r(1)) - \int_0^1 (B_0 \tilde{G}(0, s) + B_1 \tilde{G}(1, s)) A(s)r(s)ds\end{aligned} \quad (12)$$

where superscripts $+$ and $-$ denote the limits from above and below respectively. For completeness, the analogous expression for $I - HF$ is given in Appendix Appendix C.

The most straightforward way to use (12) to bound the norm of $I - FH$ is to define \tilde{G} using (9), replacing the exact quantities with $\tilde{\Phi}$ and its approximate inverse, and then use the submultiplicative property of induced matrix norms and bound each of the quantities in the Green's function individually. This leads to an estimate whose operation count scales linearly in the number of subintervals, N . If $|\Phi|$ and $|\Phi^{-1}|$ are not too large over $[0, 1]$ then this is a good strategy. However, this is often not the case, even in situations where the BVP is stable. We illustrate this phenomenon with the same test problem introduced in (6).

6.3. Behavior of the Test Problem

Consider again the simple test problem, (6). The fundamental solution and its inverse are

$$\Phi(t) = \frac{1}{\sinh(b)} \begin{pmatrix} \sinh(b-t) & \sinh(t) \\ -\cosh(b-t) & \cosh(t) \end{pmatrix}, \quad \Phi^{-1}(t) = \begin{pmatrix} \cosh(t) & -\sinh(t) \\ \cosh(b-t) & \sinh(b-t) \end{pmatrix}. \quad 8$$

While $\|\Phi\|$ is bounded, $\|\Phi^{-1}\|$ diverges as $b \rightarrow \infty$.

The general notion of BVP stability only requires the norm of the fundamental solution and of the Green's function to be small, but not the inverse of the fundamental solution. See for example [3] for details. Therefore, in general we must abandon any estimate based on bounding $\|\tilde{\Phi}\|$ and $\|\tilde{\Phi}^{-1}\|$ separately and use one based on bounding the entire Green's function. The test problem (6) does have a bounded Green's function

$$G(t, s) = \begin{cases} \frac{1}{\sinh(b)} \begin{pmatrix} \sinh(b-t) \cosh(t) & -\sinh(b-t) \sinh(t) \\ -\cosh(b-t) \cosh(t) & \cosh(b-t) \sinh(t) \end{pmatrix}, & \text{if } s \leq t \\ -\frac{1}{\sinh(b)} \begin{pmatrix} \sinh(t) \cosh(b-t) & \sinh(t) \sinh(b-t) \\ \cosh(t) \cosh(b-t) & \cosh(t) \sinh(b-t) \end{pmatrix}, & \text{if } s > t. \end{cases}$$

We emphasize that $\|G\| = \mathcal{O}(1)$ does not arise from a large cancellation of the computed results. Rather, at each endpoint the boundary conditions annihilate the growing modes of Φ^{-1} . This suggests that we should not run into the same degree of numerical cancellation issues using the BVP method as opposed to the IVP method.

7. A Sharper Bound

In this section we show how to compute a sharper bound on $\|I - FH\|$ by bounding the Green's function as a whole. Bounding the second component of $I - FH$ is straightforward so we focus on the first.

To this point the only assumption made about $\tilde{\Phi}$ and \tilde{G} is that they are piecewise C^1 . In practice, a non-rigorous numerical algorithm will provide us with approximate solution values $\tilde{\Phi}_j$ and $\tilde{G}_{i,j}$ at the centers of the intervals $[t_{i-1}, t_i]$ and rectangles $[t_{i-1}, t_i] \times [t_{j-1}, t_j]$. For example, in our computations we obtain the $\tilde{\Phi}_j$ by numerically solving the BVP and, for $i \neq j$, define

$$\tilde{G}_{i,j} = \begin{cases} \tilde{\Phi}_i B_0 \tilde{\Phi}_1 \Psi_j, & \text{if } j < i \\ -\tilde{\Phi}_i B_1 \tilde{\Phi}_N \Psi_j, & \text{if } j > i \end{cases}$$

where Ψ_j is a numerical approximation to Φ_j^{-1} . On the diagonal $i = j$ two different versions of $\tilde{G}_{i,i}$ are needed. These are denoted by

$$\tilde{G}_{i,i}^- = \tilde{\Phi}_i B_0 \tilde{\Phi}_1 \Psi_j, \quad \tilde{G}_{i,i}^+ = -\tilde{\Phi}_i B_1 \tilde{\Phi}_N \Psi_j,$$

corresponding to the lower and upper halves of the triangle respectively.

Given the values at the nodes, $\tilde{G}|_{[t_{i-1}, t_i] \times [t_{j-1}, t_j]}$ and $\tilde{\Phi}|_{[t_{j-1}, t_j]}$ are constructed to be the polynomials on each subinterval or rectangle that satisfy the equations

$$\partial_t G(t, s) = A(t)G(t, s), \quad \partial_s G(t, s) = -G(t, s)A(s), \quad G(t_{i-1/2}, t_{j-1/2}) = \tilde{G}_{i,j}$$

and

$$\Phi' = A\Phi, \quad \Phi(t_{j-1/2}) = \tilde{\Phi}_j$$

up to some order $m - 1$. Formulas for the coefficients and the ODE residual are given in Appendix Appendix D. Again, on the rectangle with $i = j$ different versions of \tilde{G} are needed, one corresponding to the upper half of the triangle and one to the lower, constructed from $\tilde{G}_{i,i}^+$ and $\tilde{G}_{i,i}^-$ respectively. The resulting $\tilde{\Phi}$ and \tilde{G} will be piecewise smooth but not continuous. This is the reason we generalized the solution space in section 4 to allow for discontinuities.

We emphasize that in the absence of jump discontinuities at the mesh points, this method reduces to a piecewise Taylor model IVP method for Φ , see for example [29].

While well suited for initial value problems, such methods perform extremely poorly for BVPs with an unstable IVP such as the examples in section 9. Therefore, having accurate $\tilde{\Phi}_j$'s as inputs is crucial to the success of the method; the Taylor series simply ensure sufficiently small error over the interior of each subinterval of the mesh.

Using Appendix Appendix D we can write $A\tilde{\Phi}(t) - \tilde{\Phi}'(t) = R_j(t)\tilde{\Phi}_{j-1}(t - t_{j-1})^m$ on each $[t_{j-1}, t_j]$, and similarly for \tilde{G} , and break the integrals in (12) into sums of integrals over the subintervals of the mesh to obtain

$$\begin{aligned}
& \|(I - FH)_1\| \\
& \leq \sum_{j=1}^N \sum_{k=1, j \neq k}^N 2h_k \frac{(h_j/2)^{m+1}}{m+1} |\tilde{G}_{j,k}| \|I + F_k(z)\|_k \|A\|_k \|R_j\|_j \\
& \quad + \sum_{j=1}^{N-1} \sum_{k=1}^N h_k |(I + E_j(t_j))\tilde{G}_{j,k} - (I + E_{j+1}(t_j))\tilde{G}_{j+1,k}| \|I + F_k(z)\|_k \|A\|_k \\
& \quad + \sum_{j=1}^N h_j \frac{(h_j/2)^{m+1}}{m+1} \left[\|\tilde{G}_{j,j}^-(I + F_j(z))\|_j + \|\tilde{G}_{j,j}^+(I + F_j(z))\|_j \right] \|A\|_j \|R_j\|_j \\
& \quad + \sum_{j=1}^N h_j \|(I + E_j(z))(\tilde{G}_{j,j}^+ - \tilde{G}_{j,j}^-)(I + F_j(z)) + I\|_j \|A\|_j \\
& \quad + \sum_{j=1}^{N-1} |(I + E_j(t_j))\Psi_j - (I + E_{j+1}(t_j))\Psi_{j+1}|(1 + |B_1|) \\
& \quad + \sum_{j=1}^N 2 \frac{(h_j/2)^{m+1}}{m+1} (1 + |B_1|) \|R_j \Psi_j\|_j,
\end{aligned} \tag{13}$$

$$\begin{aligned}
& |(I - FH)_2| \\
& \leq \sum_{j=1}^N h_j \|(B_0(I + E_1(0))\tilde{G}_{1,j} + B_1(I + E_N(1))\tilde{G}_{N,j})(I + F_j(s))\|_j \|A\|_j \\
& \quad + |I - B_0(1 + E_1(0))\Psi_1 - B_1(1 + E_N(1))\Psi_N|(1 + |B_1|),
\end{aligned} \tag{14}$$

where the subscript j on $\|\cdot\|_j$ indicates that the supremum is taken only over $[t_{j-1}, t_j]$. E_j and F_j are defined in (D.1) and (D.2) respectively. In bounding R_j on $[t_{j-1}, t_j]$ a means for analytically bounding the error term in the Taylor series expansion of $A(t)$ is needed. This can be achieved from an interval matrix valued extension for $A(t)$ and its derivatives. To bound the polynomial terms in the R_j , E_j , and F_j 's we use the simple method of summing the bounds on the norms of each monomial.

Finally, to use (11) to bound the norm of F^{-1} a machine computable bound on $\|H\|$ is needed.

$$\begin{aligned}
& \|H\| \\
& \leq \max_l \left[1 + h_l \|(1 + E_l(t))\|_l \max\{\|\tilde{G}_{l,l}^-(I + F_l(s))\|_l, \|\tilde{G}_{l,l}^+(I + F_l(s))\|_l\} \|A\|_l \right. \\
& \quad \left. + \|(1 + E_l(t))\Psi_l\|_l (1 + |B_1|) + \sum_{j=1, j \neq l}^N h_j \|(1 + E_l(t))\|_l \|\tilde{G}_{l,j}\|_l \|I + F_j(s)\|_j \|A\|_j \right].
\end{aligned} \tag{15}$$

The leading order term in N of the complexity of computing these quantities by the above formulae is $\mathcal{O}(n^3 N^2)$ where n is the dimension of the ODE system. In particular,

it does not depend on m , and so from the point of view of complexity, the degree of $\tilde{\Phi}$ can be set as high as is necessary for the Taylor series errors over the subintervals to be negligible, making the boundary conditions and jump terms the main sources of error. Parallelizing the computation of these bounds is straightforward.

These results are summarized in the following theorem.

Theorem 6. *Let Y_1 and Y_2 be defined by (7) and (8) respectively and consider the two point BVP $F[v] = (r, w)$ defined by $F : Y_1 \rightarrow Y_2$,*

$$F[v](t) = \left(v(t) - v(0) - \int_0^t A(s)v(s)ds, B_0v(0) + B_1v(1) \right)$$

where $A(t) : [0, 1] \rightarrow \mathbb{R}^{n \times n}$ is piecewise C^m on the mesh $\{t_i\}_{i=0}^N$ for some $m \geq 1$ and $B_i \in \mathbb{R}^{n \times n}$.

Let $\tilde{\Phi}$ and \tilde{G} be constructed as discussed in section 7. Define $H : Y_2 \rightarrow Y_1$ by

$$H[r, w](t) = \tilde{\Psi}(t)(w - B_1r(1)) + r(t) + \int_0^1 \tilde{G}(t, s)A(s)r(s)ds.$$

If $\|I - FH\| \leq \alpha < 1$, as computed by (13) and (14), then $F^{-1} : Y_2 \rightarrow Y_1$ exists, is bounded, and

$$\|F^{-1}\| \leq \frac{\|H\|}{1 - \alpha}.$$

8. Validated Solution of Inhomogeneous Linear BVPs

For the linear test problems presented in the following section, it will be useful to replace the Newton-Kantorovich theorem with a simpler and more explicit a posteriori error bound. Suppose we have proven $\|I - FH\| \leq \alpha < 1$ so that F is invertible. Let v be the exact solution of $F[v] = (r, w)$ and suppose we are given an approximate solution \tilde{v} . Then by (11),

$$\|v - \tilde{v}\| = \|F^{-1}[(r, w) - F[\tilde{v}]]\| \leq \|F^{-1}\| \|F[\tilde{v}] - (r, w)\| \leq \frac{\|H\|}{1 - \alpha} \|F[\tilde{v}] - (r, w)\|. \quad (16)$$

Suppose \tilde{v} is piecewise continuous on the mesh $0 = t_0 < \dots < t_N = 1$ and that $A(t)$ and $r(t)$ are piecewise C^m , hence on each subinterval $[t_{j-1}, t_j]$ we have Taylor series with remainders

$$A(t) = \sum_{l=0}^m A_l(t - t_{j-1})^l + R_j^A(t)(t - t_{j-1})^m, \quad r(t) = \sum_{l=0}^m r_l(t - t_{j-1})^l + R_j^r(t)(t - t_{j-1})^m.$$

The components of the residual in (16) can then be bounded.

$$\begin{aligned} \|(F[\tilde{v}] - (r, w))_1\| &\leq \\ &\sup_{t \in [t_{j-1}, t_j]} |\tilde{v}(t) - \tilde{v}(0) - \sum_{k=1}^{j-1} \int_{t_{k-1}}^{t_k} A_k(s)\tilde{v}(s)ds - \int_{t_{j-1}}^t A_j(s)\tilde{v}(s)ds - r_j(t)| \quad (17) \\ &+ \sum_{k=1}^j \frac{h_k^{m+1}}{m+1} \|R_k^A\|_k \|\tilde{v}\|_k + h_j^m \|R_j^r\|_j, \\ |(F[\tilde{v}] - (r, w))_2| &\leq |B_0\tilde{v}(0) + B_1\tilde{v}(1) - w| \end{aligned}$$

where, as above, $\|\cdot\|_j$ denotes the sup norm over $[t_{j-1}, t_j]$.

Similar to the approximate fundamental solution, given values \tilde{v}_j at the nodes, $\tilde{v}(t)$ is constructed on $[t_{j-1}, t_j]$ to be the polynomial

$$\tilde{v}(t) = \sum_{l=0}^m c_l (t - t_{j-1})^l, \quad c_0 = \tilde{v}_{j-1}, \quad c_{l+1} = r_{l+1} + \frac{1}{l+1} \sum_{i=\max\{0, l-m\}}^l A_i c_{l-i} \text{ for } l = 0, \dots, m-1.$$

This causes the degree 1 through m terms in (17) to vanish. We don't have the freedom to choose the zero order term; it is the analog of the jump terms from (12).

Analytically evaluating the integrals in (17), the bound on the first component of the residual becomes

$$\begin{aligned} & \| (F[v] - (r, w))_1 \| \\ & \leq \max_j \left[|\tilde{v}_{j-1} - \tilde{v}_0 - \sum_{k=1}^{j-1} \int_{t_{k-1}}^{t_k} A_k(s) \tilde{v}(s) ds - r(t_{j-1})| \right. \\ & \quad \left. + \sum_{l=m}^{2m} \frac{h_j^{l+1}}{l+1} \sum_{i=\max\{0, l-m\}}^{\min\{m, l\}} |A_i c_{l-i}| + \sum_{k=1}^j \frac{h_k^{m+1}}{m+1} \|R_k^A\|_k \|\tilde{v}\|_k + h_j^m \|R_j^r\|_j \right], \\ & \text{where } \int_{t_{k-1}}^{t_k} A_k(s) \tilde{v}(s) ds = \sum_{l=0}^{2m} \frac{h_k^{l+1}}{l+1} \sum_{i=\max\{0, l-m\}}^{\min\{m, l\}} A_i c_{l-i}. \end{aligned}$$

The bound is now in a form that can easily be programmed for automated rigorous evaluation using interval arithmetic or estimation in traditional floating point. We also note that the cost is just $\mathcal{O}(N)$ as opposed to the $\mathcal{O}(N^2)$ cost of bounding $\|F^{-1}\|$.

9. Numerical Tests

In (13) and (15) bounds were given on $\|I - FH\|$ and $\|H\|$ that involve finitely representable objects and finite operations with which we can perform validated computations, namely the piecewise polynomials $\tilde{\Phi}(t)$ and $\tilde{G}(t, s)$ and the interval valued extension of $A(t)$ and its derivatives. For rigorous bounds, we implemented this using the MATLAB interval analysis package INTLAB [32] by creating simple routines that perform algebraic operations with polynomials whose coefficients are interval matrices. With such functionality, the code that produces the desired bound on $\|I - FH\|$ is a simple translation of (13) and (14).

In this section, the applicability and accuracy of the BVP method is assessed using a pair of singularly perturbed test problems, taken from [19], as well as a nonlinear example, the existence of a periodic orbit in the Lorenz system.

To obtain usable bounds, even the exponentially small parts of the approximate fundamental solution need to be resolved with the same relative accuracy as the larger portions, otherwise the loss of accuracy will prevent the growing modes from being annihilated when forming the approximate Green's function. For problems with quickly decaying modes, the absolute tolerance of the non-rigorous solver must be set near the underflow limit in order to achieve this. This is done in the first two test problems.

Tests were performed using a uniform mesh. There is likely room for improvement by intelligently selecting the mesh but we did not employ such methods here. In table 1 the mesh size was chosen by adding points until the error approximately stabilized.

9.1. Example 1: Turning Point

Our first test problem is a singularly perturbed Airy equation

$$\epsilon v'' - (t - 1/2)v = 0, \quad v(0) = v(1) = 1,$$

Example	ϵ	N	input error	$\ I - FH\ $	solution error bound
Turning Point	10^{-4}	230	1.4×10^{-12}	5.2×10^{-9}	3.1×10^{-10}
	10^{-5}	250	5.1×10^{-8}	6.1×10^{-5}	1.2×10^{-4}
	10^{-6}	600	2.2×10^{-6}	3.6×10^{-3}	4.0×10^{-4}
Potential Barrier	10^{-5}	350	6.0×10^{-8}	7.0×10^{-6}	8.7×10^{-4}
	10^{-6}	600	3.9×10^{-8}	1.8×10^{-4}	1.3×10^{-4}

Table 1: Test results for the BVP method on the example problems.

which is a model of the quantum mechanical wave function near a turning point in the potential, here at $t = 1/2$. The exact solution is a linear combination of Airy functions and is shown in figure 1, where $\epsilon = 10^{-6}$. The solution exhibits dense oscillations for $t < 1/2$ and a boundary layer near $t = 1$. We used the BVP method in the cases $\epsilon = 10^{-4}, 10^{-5}, 10^{-6}$.

We used $m = 15$ with the aim of making the Taylor series and approximate inverse errors negligible, allowing us to focus on how the error in the initial approximation supplied to the BVP method translates into the bound produced by the method.

If we let err_j^i be the i th component of the j th jump error from (17) then the weight used in this test has diagonal elements given by

$$w_i \sum_j |\text{err}_j^i| = \text{constant}, \quad \max_i w_i = 1.$$

This choice prevents overestimation of the error in certain components when they have widely different scales and makes a large difference in the quality of the bounds, up to several orders of magnitude; it was often the difference between the existence test $\|I - FH\| < 1$ passing or failing. Since the jump errors can be computed in $\mathcal{O}(N)$ operations prior to the main $\mathcal{O}(N^2)$ computation, this is an effective and practical way to improve the estimates.

The test results are shown in table 1. The fourth column gives the error in solution values on the mesh that are provided to the BVP method, the fifth column is the bound on $\|I - FH\|$ computed by the method, and the final column is the computed bound on the absolute value of the error in v .

The a posteriori BVP method does overestimate the error by several orders of magnitude, but the error bounds are still practical. The IVP fundamental solution method would not be usable in this situation, as the fundamental solution matrix has a norm $|Y(1)| \approx 10^{12}$ for $\epsilon = 10^{-4}$. The use of an adaptive weighted norm is crucial for the success of the method and greatly improves the error bounds. Without the weight, the existence test $\|I - FH\| < 1$ fails even at $\epsilon = 10^{-5}$.

The BVP method fails on this problem for $\epsilon = 10^{-7}$, as Φ becomes so ill conditioned that its decaying components cannot be resolved to sufficient relative accuracy due to underflow. This point will reappear in the subsequent example as well; the exponentially decaying modes of Φ (which tend to be the least ‘interesting’ features) cause the most trouble for the BVP method. In other words, while a large norm for the inverse fundamental solution does not impact BVP stability, over/underflow issues mean that it is still the main limiting factor of the BVP method in its current form. However, the problem is much less severe than ill conditioning in the IVP method.

9.2. Example 2: Potential Well

As a second test, consider a quantum mechanical potential well problem

$$\epsilon v'' + ((t - 1/2)^2 - \omega^2)v = 0, \quad v(0) = 1, \quad v(1) = 2$$

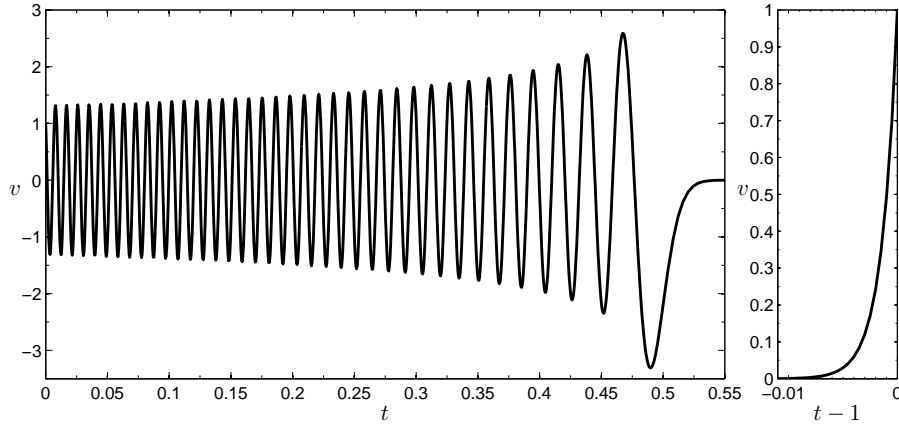


Figure 1: Exact solution to the turning point problem for $\epsilon = 10^{-6}$. For $t < 1/2$ the system is oscillatory (left) and it has a boundary layer near $t = 1$ (right).

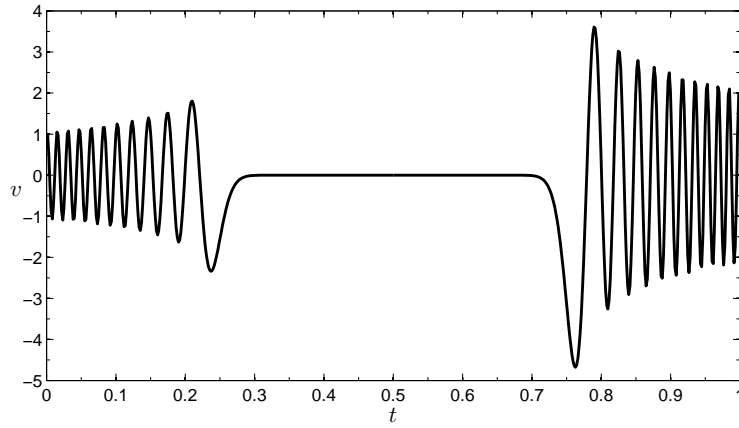


Figure 2: Solution to the potential problem for $\epsilon = 10^{-6}$ (right).

where we take $\omega = 1/4$. The solution is oscillatory on $[0, 1/4] \cup [3/4, 1]$ and exponentially decaying as one moves towards the center of $[1/4, 3/4]$ as seen in figure 2 (right pane) for $\epsilon = 10^{-6}$. We used $m = 15$ and the same formula for W as in the prior example. Again, the method fails once the decaying modes start to underflow, which occurs for $\epsilon = 10^{-7}$.

For this example we don't have an analytical formula for the exact solution, so the input error reported for in table 1 for this problem is obtained by comparing approximate solution values after refining the mesh. In the first two examples, the supremum norm of the exact solution was relatively consistent between the different parameter values, but that is not true for the current example, where $\|v\| \approx 300$ for $\epsilon = 10^{-5}$ and is single digits $\epsilon = 10^{-6}$. This explains why the absolute error is so similar for the cases tested despite the difference in ϵ .

9.3. Example 3: Lorenz System

As our final example, we study a non-linear problem, the existence of periodic solutions to the Lorenz system. Scaling the independent variable by the (unknown) period T , the BVP is

$$x' = T\sigma(y - x), \quad y' = Tx(\rho - z) - y, \quad z' = T(xy - \beta z), \quad T' = 0$$

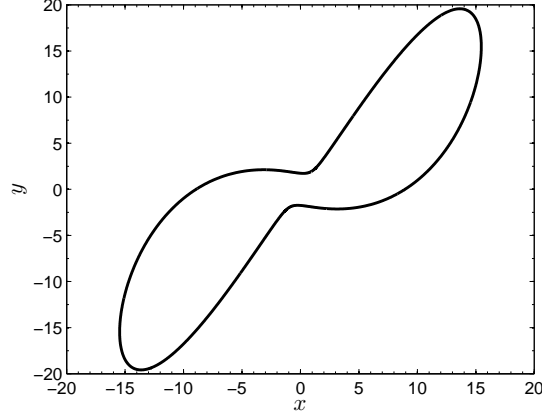


Figure 3: Periodic orbit for the Lorenz system, projected onto the x - y plane.

$$x(0) = x(1), \quad y(0) = y(1), \quad z(0) = z(1).$$

In order to fix the initial point on the periodic orbit an additional boundary condition is needed, which we take to be

$$x(0) = y(0), \text{ i.e. } x'(0) = 0. \quad (18)$$

Let $f, g : \mathbb{R}^4 \rightarrow \mathbb{R}^4$ denote the vector field and boundary conditions respectively and G be the corresponding BVP operator, defined as in (4).

In [5, 13], computer aided proof techniques were used to show existence of periodic orbits to the Lorenz system. In particular, in [5] existence was shown for parameter values

$$\sigma = 10, \quad \beta = 8/3, \quad \rho = 28$$

and initial conditions and period T close to

$$x(0) \approx -12.78619, \quad y(0) \approx -19.36419, \quad z(0) \approx 24, \quad T \approx 1.559.$$

Note that our initial point on the orbit, defined by (18), differs from the above initial conditions. We will test our method on this same orbit, shown in the x - y plane in figure 3.

A Taylor series approximation to the solution centered at $t_{i-1/2}$ can be derived

$$x(t) = \sum_{j=0}^m x_j (t - t_{i-1/2})^j, \quad y(t) = \sum_{j=0}^m y_j (t - t_{i-1/2})^j, \quad z(t) = \sum_{j=0}^m z_j (t - t_{i-1/2})^j, \quad T),$$

$$x_{r+1} = \frac{1}{r+1} T \sigma (y_r - x_r), \quad y_{r+1} = \frac{1}{r+1} T (\rho x_r - y_r - \sum_{j=0}^r x_j z_{r-j}),$$

$$z_{r+1} = \frac{1}{r+1} T (\sum_{j=0}^r x_j y_{r-j} - \beta z_r),$$

where x_0, y_0, z_0 , and T are obtained from numerical approximations to the periodic orbit at the centers of the mesh intervals $[t_{i-1}, t_i]$.

The Jacobian of the Lorenz system vector field f can be Taylor expanded

$$\begin{aligned}
& D_y f(t, x, y, z, T) \\
&= \begin{pmatrix} -T\sigma & T\sigma & 0 & \sigma(y_0 - x_0) \\ T(\rho - z_0) & -T & -Tx_0 & x_0(\rho - z_0) - y_0 \\ Ty_0 & Tx_0 & -T\beta & x_0y_0 - \beta z_0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
&+ \sum_{j=1}^m \begin{pmatrix} 0 & 0 & 0 & \sigma(y_j - x_j) \\ -Tz_j & 0 & -Tx_j & \rho x_j - y_j - \sum_{k=0}^j x_k z_{j-k} \\ Ty_j & Tx_j & 0 & -\beta z_j + \sum_{k=0}^j x_k y_{j-k} \\ 0 & 0 & 0 & 0 \end{pmatrix} (t - t_{i-1/2})^j \\
&+ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sum_{r=m+1}^{2m} (t - t_{i-1/2})^r \sum_{j=r-m}^m x_j z_{r-j} \\ 0 & 0 & 0 & \sum_{r=m+1}^{2m} (t - t_{i-1/2})^r \sum_{j=r-m}^m x_j y_{r-j} \\ 0 & 0 & 0 & 0 \end{pmatrix}.
\end{aligned}$$

Combined with theorem 6, this can be used to compute upper bounds on the values of the parameters β , K , η that appear in the Newton-Kantorovich theorem, see Appendix A. The trivial weight $W = I$ was used in this test. Denote the piecewise polynomial approximate solution by y_0 , let $F = DG(y_0)$, and H be its approximate inverse as in Theorem 6. Using $m = 15$, an equally spaced mesh of size $N = 35$, and a domain $D = B_\epsilon(y_0)$, $\epsilon \approx 2.3 \times 10^{-4}$, our method provides a rigorous existence proof with the following parameters

$$\begin{aligned}
& \|G(y_0)\| \leq 1.5 \times 10^{-10}, \quad \|I - FH\| \leq 0.19, \quad \|F^{-1}\| \leq 1.1 \times 10^5, \\
& K = 8 \times 10^{-2}, \quad s_0 \leq 1.8 \times 10^{-5}, \quad s_1 \geq 2.1 \times 10^{-4}.
\end{aligned}$$

In other words, a solution exists within a ∞ -norm ball of radius s_0 about the approximate solution and the solution is unique within the ball of radius s_1 .

The computation was done in MATLAB using the interval arithmetic package INT-LAB [32] on a 2GHz Intel Core i7 and took 142 seconds. This includes the time to compute the approximate solution y_0 and approximate BVP fundamental solution $\tilde{\Phi}$. These were computed using the MATLAB routines ode15s and bvp5c with absolute and relative error tolerances of 10^{-9} .

10. Conclusion

We have presented an a posteriori method for proving existence to and deriving rigorous error bounds for two point boundary value problems on a finite interval, summarized in Theorem 6. The method applies to general n -dimensional systems without any assumption on the form of the vector field. It uses a (non-rigorous) approximation to the Green's function of the BVP to generate the bounds and can be evaluated using interval arithmetic for mathematically rigorous results or in traditional floating point for faster generation of approximate bounds. Because the method is based on the Green's function of a BVP rather than the fundamental solution to an IVP, the method is applicable to cases where the BVP is stable but the corresponding IVP is unstable. An adaptively chosen weight matrix was used in some of the norms. This improves the quality of the final L^∞ error bounds by several orders of magnitude in many of the tests.

In section 9 we tested the BVP method on a pair of singularly perturbed linear problems that exhibit such problematic features as dense oscillation and boundary layers. The method is successful in proving existence and producing reasonable and usable error bounds, even when the relevant perturbation parameter becomes moderately small. We

have also successfully applied it to rigorously prove the existence of a periodic orbit in the Lorenz system.

In the cases tested, the main limiting factor on the success of the method is the extreme ill conditioning of the approximate BVP fundamental solution Φ as the parameter that controls the singular perturbation is made smaller. Although Φ itself has moderate sized norm in the tests, it is close to being singular. The BVP method requires computation of the fundamental solution and its inverse to sufficient *relative accuracy*; poorly resolved decaying modes will spoil the method and the method always fails once the underflow limit is reached. This commonly occurs for very stiff problems and so, while the BVP method works for moderately stiff problems as we have shown, it fails in the very stiff limit. This issue could likely be addressed in a brute force manner by employing an interval or floating point arithmetic package that allows for exponent values of substantially larger magnitude than are allowed in standard floating point arithmetic, but we did not employ such a technique here.

Appendix A. Newton-Kantorovich Theorem

For convenience, in this appendix we state a version of the Newton-Kantorovich theorem that was used above.

Theorem 7 (Newton-Kantorovich Theorem). *Let X, Y be Banach spaces, $D \subset X$ be open and convex, $F : D \rightarrow Y$ be differentiable, and*

$$\|DF(x) - DF(y)\| \leq K\|x - y\|$$

in D . Let $y_0 \in D$ and $DF(y_0)$ have bounded inverse A .

Suppose $\beta \geq \|A\|$, $\eta \geq \|AF(y_0)\|$, and $h \equiv \beta K \eta \leq 1/2$. Set

$$s_0 = \frac{1}{\beta K}(1 - \sqrt{1 - 2h}), \quad s_1 = \frac{1}{\beta K}(1 + \sqrt{1 - 2h}).$$

Suppose $S \equiv \overline{B_{s_0}(y_0)} \subset D$. Then the Newton iteration is well defined, lies in S and converges to $x \in S$, a solution of $F(x) = 0$. This is the unique solution in $D \cap B_{s_1}(y_0)$.

In the above, η is computed by bounding $\|A\|\|F(y_0)\|$.

Appendix B. Computing $I - FH$

In this appendix a formula is derived for $I - FH$. The goal is decompose it into several terms, each of which obviously vanishes when $\tilde{\Phi}$ and \tilde{G} equal the exact fundamental solution Φ and Green's function G , respectively. The calculation is long but relatively straightforward. We outline the key steps below.

First, using the definitions of H and F and taking $t \notin \{t_i\}_{i=0}^N$ the two components equal

$$\begin{aligned} & (I - FH)[r, w]_1(t) \\ &= \tilde{\Phi}(0)(w - B_1 r(1)) + \int_0^1 \tilde{G}(0, s) A(s) r(s) ds - \tilde{\Phi}(t)(w - B_1 r(1)) \\ & \quad - \int_0^1 \tilde{G}(t, s) A(s) r(s) ds + \int_0^t A(s) \tilde{\Phi}(s) ds (w - B_1 r(1)) + \int_0^t A(s) r(s) ds \\ & \quad + \int_0^t A(s) \int_0^1 \tilde{G}(s, z) A(z) r(z) dz ds, \\ & (I - FH)[r, w]_2 \\ &= [I - B_0 \tilde{\Phi}(0) - B_1 \tilde{\Phi}(1)](w - B_1 r(1)) - \int_0^1 (B_0 \tilde{G}(0, s) + B_1 \tilde{G}(1, s)) A(s) r(s) ds. \end{aligned}$$

One can check that

$$\begin{aligned} B_0 G(0, s) + B_1 G(1, s) &= (-B_0 \Phi(0) B_1 \Phi(1) + B_1 \Phi(1) B_0 \Phi(0)) \Phi^{-1}(s) \\ &= -(B_0 \Phi(0) + B_1 \Phi(1) - I) B_1 \Phi(1) + B_1 \Phi(1) (B_0 \Phi(0) + B_1 \Phi(1) - I). \end{aligned}$$

It is apparent that each term vanishes for the exact solution.

As for the first component, we introduce $\tilde{\Phi}'$ and $\partial_t \tilde{G}(t, s)$ to obtain terms that vanish when the ODE is satisfied

$$\begin{aligned} &(I - FH)[r, w]_1(t) \\ &= \tilde{\Phi}(0)(w - B_1 r(1)) + \int_0^1 \tilde{G}(0, s) A(s) r(s) ds - \tilde{\Phi}(t)(w - B_1 r(1)) - \int_0^1 \tilde{G}(t, s) A(s) r(s) ds \\ &\quad + \int_0^t -\tilde{\Phi}'(s) + A(s) \tilde{\Phi}(s) ds (w - B_1 r(1)) + \int_0^t \tilde{\Phi}'(s) ds (w - B_1 r(1)) + \int_0^t A(s) r(s) ds \\ &\quad + \int_0^t \int_0^1 (-\partial_s \tilde{G}(s, z) + A(s) \tilde{G}(s, z)) A(z) r(z) dz ds + \int_0^t \int_0^1 \partial_s \tilde{G}(s, z) A(z) r(z) dz ds. \end{aligned}$$

Now integrate by parts, taking into account the discontinuities of $\tilde{\Phi}(s)$ and $\tilde{G}(s, t)$ at $s = t_i$ as well as $\tilde{G}(s, t)$ at $s = t$. After substantial simplification we arrive at

$$\begin{aligned} &(I - FH)[r, w]_1(t) \tag{B.1} \\ &= - \int_0^t \tilde{\Phi}'(s) - A(s) \tilde{\Phi}(s) ds (w - B_1 r(1)) + \int_0^t (\tilde{G}(z^-, z) - \tilde{G}(z^+, z) + I) A(s) r(s) ds \\ &\quad + \sum_{j=1}^{j_t} (\tilde{\Phi}(t_j^-) - \tilde{\Phi}(t_j^+)) (w - B_1 r(1)) + \int_0^1 \left[\sum_{j=1}^{j_t} (\tilde{G}(t_j^-, z) - \tilde{G}(t_j^+, z)) \right] A(z) r(z) dz \\ &\quad - \int_0^t \int_0^1 (\partial_s \tilde{G}(s, z) - A(s) \tilde{G}(s, z)) A(z) r(z) dz ds \end{aligned}$$

where j_t is the smallest index with $t_j < t$ and the superscripts $+$ and $-$ denote limits from above and below respectively.

The exact Greens function satisfies

$$G(t^+, t) - G(t^-, t) = \Phi(t) (B_1 \Phi(1) + B_0 \Phi(0)) \Phi^{-1}(t) = I$$

and is continuous away from the boundary. The exact fundamental solution Φ is continuous as well. Therefore, if $\tilde{\Phi}$ and \tilde{G} equal the exact fundamental solution Φ and Green's function G then the jump terms in (B.1) vanish. The remaining terms are zero since Φ and G satisfy the ODE. Therefore we have succeeded in putting $I - FH$ into a form where each term is manifestly zero when using the exact solution. This suggests that a reasonable bound on $\|I - FH\|$ might be obtained by bounding each of these terms individually, as done in section 7.

Appendix C. Formula for $I - HF$

A similar procedure to Appendix Appendix B yields a formula for $I - HF$. For $t \notin \{t_i\}_{i=0}^N$

$$\begin{aligned}
& (I - HF)[v](t) \\
&= \int_0^1 \left(\frac{\partial}{\partial s} \tilde{G}(t, s) + \tilde{G}(t, s)A(s) \right) \left(v(0) + \int_0^s A(r)v(r)dr \right) ds \\
&+ (\tilde{G}(t, 0) - \tilde{\Phi}(t)B_0)v(0) - (\tilde{G}(t, 1) + \tilde{\Phi}(t)B_1) \left(v(0) + \int_0^1 A(s)v(s)ds \right) \\
&- \sum_{j=1}^{N-1} \left(\tilde{G}(t, t_j^-) - \tilde{G}(t, t_j^+) \right) \left(v(0) + \int_0^{t_j} A(r)v(r)dr \right) \\
&- \left(\tilde{G}(t, t^-) - \tilde{G}(t, t^+) - I \right) \left(v(0) + \int_0^t A(r)v(r)dr \right)
\end{aligned}$$

where $j_t^- = \max\{j : t_j < t\}$ and $j_t^+ = \min\{j : t_j > t\}$. The most significant difference is that the jump terms now involve the second argument of \tilde{G} . In practice we found that the bounds obtained using $I - FH$ to be tighter than those using $I - HF$ and so we have based the BVP method on $I - FH$, but the other choice could have been made and may be preferable in some cases.

Appendix D. Approximate Solution

As discussed above, the data for the BVP method consists of sets $\tilde{\Phi}_j$ and $\tilde{G}_{i,j}$ of approximations to the fundamental solution Φ and Green's function G at the centers of the intervals $[t_{i-1}, t_i]$ and rectangles $[t_{i-1}, t_i] \times [t_{j-1}, t_j]$. These need to be extended to C^1 functions on each interval or rectangle. This is done by letting $I + E_i(t)$, $I + F_j(t)$ be the polynomials of degree $m \geq 1$ that satisfies the ODEs

$$\begin{aligned}
\frac{d}{dt}E_i(t) &= A(t)(I + E_i(t)), \quad E_i(0) = 0, \\
\frac{d}{dt}F_j(t) &= -(I + F_j(t))A(t), \quad F_j(0) = 0
\end{aligned}$$

up to order $m - 1$. The functions

$$\tilde{\Phi}(t)|_{[t_{i-1}, t_i]} = (I + E_i(t))\tilde{\Phi}_i, \quad \tilde{G}(t, s)|_{[t_{i-1}, t_i] \times [t_{j-1}, t_j]} = (I + E_i(t))\tilde{G}_{i,j}(I + F_j(s))$$

are then approximate solutions to the ODEs satisfied by Φ and G . Note that on the rectangle with $i = j$ two different versions are needed, one corresponding to the upper half of the triangle and one to the lower, constructed from $\tilde{G}_{i,i}^+$ and $\tilde{G}_{i,i}^-$ respectively, where

$$\tilde{G}_{i,i}^- - \tilde{G}_{i,i}^+ = I.$$

Recursive formulas for the coefficients are given below. We suppose the coefficient matrix $A(t)$ is C^m and write the Taylor series with remainder about $t_{j-1/2}$ as

$$A(t) = \sum_{k=0}^{m-1} A_k(t - t_{j-1/2})^k + r_m(t)(t - t_{j-1/2})^m.$$

Define E_j, F_j on $[t_{j-1}, t_j]$ by

$$I + E_j(t) = \sum_{k=0}^m (t - t_{j-1/2})^k E_j^k, \quad E_j^0 = I, \quad E_j^k = \frac{1}{k} \sum_{l=0}^{k-1} A_l E_j^{k-l-1}, \quad (\text{D.1})$$

$$I + F_j(t) = \sum_{k=0}^m (t - t_{j-1/2})^k F_j^k, \quad F_j^0 = I, \quad F_j^k = -\frac{1}{k} \sum_{l=0}^{k-1} F_j^{k-l-1} A_l \quad (\text{D.2})$$

where $t_{j-1/2}$ denotes the midpoint of $[t_{j-1}, t_j]$. Note that these quantities do not involve the remainder term $A_m \equiv r_m(t)$.

With these, the ODE residuals are

$$A(t)(I + E_j(t)) - E_j'(t) = \sum_{k=m}^{2m} (t - t_{j-1/2})^k \sum_{l=0}^m A_l E_j^{k-l} \equiv R_j(t)(t - t_{j-1/2})^m,$$

$$F_j'(t) + (I + F_j(t))A(t) = \sum_{k=m}^{2m} (t - t_{j-1/2})^k \sum_{l=0}^m F_j^{k-l} A_l.$$

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